

Existence of solitary solutions in nonlinear chains

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Techniques for examining the existence and stability of localized modes are presented. The methods are demonstrated in detail for a discrete nonlinear Schrödinger (DNS) equation, but also apply to other systems, e.g., the discrete nonlinear Klein-Gordon (DNKG) equation. Stationary states may be found via variational principles or through generating functions. The latter technique makes use of solutions of a continuous difference-equation and allows for localized modes with different symmetry properties. It is shown that several families of stationary solutions exist, and a constructive procedure to calculate the latter is presented. In the case of the DNS equation, an analytical stability criterion for symmetric solitons (N -theorem) proves that the discrete equation exhibits localization in regimes where blow-up cannot occur in the continuum analog. Stable nonlinear solutions are found for the DNKG equation. The analytical calculations are supplemented by numerical simulations. [S1063-651X(96)11309-X]

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I. INTRODUCTION

In continuous systems it is well-known [1–5] that as a result of balance between nonlinear and dispersive effects specific nonlinear objects, namely solitary waves, may appear. The one-dimensional cubic nonlinear (continuous) Schrödinger equation is a paradigm for soliton bearing equations and one of the most useful physical models of nonlinear science. Since it can be solved by the inverse scattering transform, in principle all of its rich dynamical behavior is known. The situation is different for discrete systems. Here, not so many results are known analytically, except for the integrable form invented by Ablowitz and Ladik [6]. However, the integrable discrete cubic nonlinear Schrödinger equation does not appear in physically motivated models [7–11], such as coupled nonlinear atomic strings, arrays of coupled optical wave guides, proton dynamics in hydrogen-bonded chains, the Davydov and Holstein models for transport of excitation energy in biophysical systems, Scheibe aggregates, the Hubbard model, electrical lattices, DNA dynamics, molecular crystals, and so on.

Nonlinear localized modes in discrete systems have been a subject of intense but mainly numerical investigations during recent years [12–21]. Different types of localized states were found, and very elegant and efficient schemes have been developed for calculating solitary wave solutions. The broad and discrete solutions may be approximated by the corresponding continuum solutions, but there exist other types of discrete modes that definitely will not obey the continuum limit. Some of the latter show stable behavior in numerical experiments. However, from the principle point of view, numerical simulations cannot prove stability in the strict sense. Thus, analytical or at least semianalytical criteria are strongly needed, and it is the primary motivation of this paper to develop systematic analytical methods for examining the existence and stability of solitary wave solutions in discrete nonlinear systems.

When studying existence and stability [22–24] of discrete solitary waves one immediately recognizes that the underlying spectral problems are strongly related. The latter depend

on the boundary conditions, parity requirements, nonlinear potentials, and last but not least, the structure of the system under consideration. Although it is possible to propose some general strategy being independent of the actual system [25], its evaluation always requires some modifications when a specific problem is investigated. Thus, when we present some additional methods for existence of discrete solitary waves, we shall demonstrate them on a specific example, i.e., the discrete nonlinear Schrödinger (DNS) equation, but one should have in mind that they should be applicable also to other systems, e.g., the discrete nonlinear Klein-Gordon (DNKG) equation. After the detailed description and exemplification for one equation (DNS), one should be able to apply the procedure immediately to other systems being of interest. Our brief consideration of the DNKG equation should be interpreted as a first step in this direction.

We choose a DNS equation with arbitrary power nonlinearity because of the following reason [26–29]. The continuous one-dimensional nonlinear Schrödinger equation also possesses solitary wave solutions when its power nonlinearity is changed from cubic to other algebraic forms. Such different types of nonlinearities might appear for at least two reasons. (i) The physical model may require a strong anharmonic coupling which does not result in a cubic nonlinearity. The latter is a characteristic of the integrable Schrödinger equation. (ii) From the mathematical point of view, it may be advisable to raise the exponent of the (cubic) power nonlinearity in order to mimic the multidimensional behavior of the Schrödinger model. Solitary wave solutions of a one-dimensional continuous nonlinear Schrödinger equation with arbitrary power nonlinearity can be stable (corresponding, e.g., to the stable solitons) or unstable. The latter means that dispersion balances nonlinear steepening only in the stationary case. Small perturbations around the solitary wave may break this balance leading to instability and perhaps collapse. Because of that rich dynamical behavior, our DNS model will be the exact discrete analog of the general continuous nonlinear Schrödinger equation.

The first area concerns the *existence* of discrete solitary wave solutions. Let us, for a moment, consider the con-

tinuum nonlinear Schrödinger equation

$$i \partial_t \psi + \partial_x^2 \psi + (\sigma + 1) |\psi|^{2\sigma} \psi = 0. \tag{1}$$

This equation reduces for $\sigma = 1$ to the famous cubic nonlinear Schrödinger equation. At this stage we would like to mention that in the following we shall always consider the focusing case [with a plus sign in front of the nonlinearity of Eq. (1)], but all the considerations will also work in the defocusing case. The (continuous) Schrödinger equation (1) possesses, for arbitrary power nonlinearities, stationary solitary wave solutions. If we introduce

$$\psi(x, t) \equiv G(x) \exp(i \eta^2 t), \tag{2}$$

with the stationary envelope $G(x)$ and a nonlinear frequency shift η^2 , stationary localized solutions of Eq. (1) can be presented explicitly, i.e.,

$$G(x) = \eta^{1/\sigma} \operatorname{sech}^{(1/\sigma)}[\sigma \eta(x - x_0)], \tag{3}$$

where x_0 is a free parameter. When we now turn to a discrete version of Eq. (1) (which will be the main object of demonstration in this paper),

$$i \partial_t \psi_j + \psi_{j+1} - 2 \psi_j + \psi_{j-1} + (\sigma + 1) |\psi_j|^{2\sigma} \psi_j = 0 \tag{4}$$

for $j = 0, \pm 1, \pm 2, \dots$ and with boundary conditions $|\psi_j| \rightarrow 0$ for $|j| \rightarrow \infty$ the situation has completely changed. We do not know analytically any nontrivial (localized) solitary wave solution. Of course, numerically solutions have been found (also for finite systems with Dirichlet or periodic boundary conditions). We shall discuss some strategy to construct stationary solutions of Eq. (4) in the form

$$\psi_j = G_j \exp(i \lambda t) \tag{5}$$

in the next section.

Let us emphasize another qualitative difference between Eqs. (1) and (4). Even in the nonintegrable case $\sigma \neq 1$, Eq. (1) possesses three constants of motion,

$$N_0^2(\psi) := \int_{-\infty}^{+\infty} dx |\psi|^2, \tag{6}$$

$$P(\psi) := i \int_{-\infty}^{+\infty} dx \psi \partial_x \psi^* + \text{c.c.}, \tag{7}$$

$$H(\psi) := \int_{-\infty}^{+\infty} dx [|\partial_x \psi|^2 - |\psi|^{2\sigma+2}], \tag{8}$$

reflecting conservation of particle number, momentum, and energy, respectively. (In the integrable case $\sigma = 1$ we have an infinite number of independent conserved quantities.) Now, in the discrete situation (4) translation symmetry is broken, and no conserved analog to P exists. Instead, we only have two constants of motion:

$$N_0^2(\psi) := \sum_{j=-\infty}^{\infty} |\psi_j|^2, \tag{9}$$

$$H(\psi) := \sum_{j=-\infty}^{\infty} [|\psi_{j+1} - \psi_j|^2 - |\psi_j|^{2\sigma+2}]. \tag{10}$$

Note that Eq. (4) can be written in Hamiltonian form

$$i \dot{\psi}_n = \frac{\partial H}{\partial \psi_n^*}, \tag{11}$$

showing that it is still conservative. However, the lack of conservation of momentum has severe consequences for the existence of localized solutions. For example, we do not expect a continuous free parameter like x_0 . Moreover, in the continuum case (1), Galilei invariance [$X = x - Vt, T = t$] produces from Eq. (2) the whole set of solutions

$$\begin{aligned} \psi_V(X, T) = & \left(\eta^2 + \frac{1}{4} V^2 \right)^{1/2\sigma} \operatorname{sech}^{(1/\sigma)} \left[\sigma \left(\eta^2 + \frac{1}{4} V^2 \right)^{1/2} X \right] \\ & \times \exp(i \eta^2 T + i V X / 2). \end{aligned} \tag{12}$$

We do not have an equivalent class of solutions in the discrete case.

We can also view this problem from another viewpoint. When introducing into the stationary form of Eq. (4), i.e.,

$$G_{j+1} - 2G_j + G_{j-1} = \lambda G_j - (\sigma + 1) |G_j|^{2\sigma} G_j, \tag{13}$$

the abbreviation $\Theta_n := G_n$, and defining $J_{n+1} := \Theta_{n+1} - \Theta_n$, we can rewrite Eq. (13) in the form of a *generalized standard mapping*

$$J_{n+1} = J_n + f^*(\Theta_n), \tag{14}$$

$$\Theta_{n+1} = \Theta_n + J_{n+1}, \tag{15}$$

with

$$f^*(\Theta_n) := \lambda \Theta_n - (\sigma + 1) |\Theta_n|^{2\sigma} \Theta_n. \tag{16}$$

Imaginating the rich and complicated ‘‘dynamics’’ inherent in such types of mappings, we get a feeling for the problems encountered when trying to find analytical solutions. Thus, any progress in this respect will be very helpful.

Besides existence, *stability* problems are next urgent to be solved. Again let us motivate the idea by comparing with the continuum case (1). For the latter, a virial theorem can be derived,

$$\partial_t^2 \int dx x^2 \psi \psi^* = 8H + 4(2 - \sigma) \int dx |\psi|^{2\sigma+2}. \tag{17}$$

There is no hope to derive a similar virial theorem in the discrete case (4). In the continuous case it has been shown that for $\sigma \geq 2$ (stationary) solitary wave solutions become unstable under small perturbations. The question, however, arises whether $\sigma = 2$ is also a ‘‘critical’’ exponent in the discrete situation. We shall comment on that in the second part of the paper.

The whole manuscript is organized as follows. In the next section we comment on variational principles for the existence of solutions. We shall favor one principle which will work systematically for symmetric solutions and which has a form being suitable for stability considerations. As has been

indicated already, we shall obtain only some ground states by that procedure. In Sec. III we show, by introducing generating functions, that several families of stationary solutions do exist. A constructive procedure for calculating the various members of different families is presented. Section IV is devoted to stability considerations. For the (symmetric) ground states, a so-called N -theorem is derived which allows us to determine stability with respect to a certain class of symmetric perturbations. In addition to the analytical tools, in the general case we also have to rely on numerical simulations. The latter are especially useful for following the non-linear developments of linearly unstable modes. After having demonstrated the methods for a DNS equation, with results for the latter, we briefly turn to a second example in order to show that the procedure is general enough to be useful for several discrete systems. In Sec. V, results for a DNKG equation are presented. The paper is concluded by a short summary and outlook.

II. GROUND STATES FROM VARIATIONAL PRINCIPLES

The aim of this section is to obtain solutions of Eq. (13) by a variational approach. First we comment on the simple case of a finite chain with $2N+1$ oscillators and periodic boundary conditions. One may be tempted to believe that the following procedure is the most promising one: Minimizing $H(\psi)$ under the constraint of fixed $N_0^2(\psi)$. An obvious advantage of this approach would be a simultaneous proof of stability. Note that for fixed N_0^2 , H is bounded from below:

$$H \geq -\max |\psi_n|^{2\sigma} N_0^2 \geq -N_0^{\sigma+2}. \quad (18)$$

In case of finite N_0^2 the minimum will be attained on some state being evidently stable with respect to perturbations yielding the same value of N_0^2 . When accepting this procedure, λ plays the role of a Lagrange multiplier which has to be determined from the constraint $N_0^2 = \text{const}$. But in this way one has problems to show that the Lagrange parameter λ can attain arbitrary continuous values $\lambda = \eta^2$. This difficulty is a consequence of the absence of scaling invariance in the discrete situation.

An alternative is to minimize

$$W(\psi) = \sum_{n=-N}^N [|\psi_{n+1} - \psi_n|^2 + \lambda |\psi_n|^2] \quad (19)$$

under the constraint

$$I(\psi) = \sum_{n=-N}^N |\psi_n|^{2\sigma+2} = \text{const}. \quad (20)$$

We assume in the following that — besides a frequency shift factor $\exp(i\lambda t)$ — the stationary states (G_n) are real valued.

The first variation of W leads to

$$-\tilde{G}_{i+1} + 2\tilde{G}_i - \tilde{G}_{i-1} + \lambda \tilde{G}_i - \mu(\sigma+1)\tilde{G}_i^{2\sigma+1} = 0, \quad (21)$$

where μ is the Lagrangian multiplier. Multiplying by \tilde{G}_i and summing up over i results in

$$\sum_i (\tilde{G}_{i+1} - \tilde{G}_i)^2 + \lambda \sum_i \tilde{G}_i^2 = \mu(\sigma+1) \sum_i \tilde{G}_i^{2\sigma+2}. \quad (22)$$

Thus $\mu > 0$ for $\lambda > 0$ (which is the case we are interested in). Defining $G_i = \mu^{1/2\sigma} \tilde{G}_i$ we get for the first variation

$$\delta W = \sum_{i=-N}^N \delta \psi_i (H_+ G)_i = 0, \quad (23)$$

i.e., $(H_+ G)_i = 0$ with

$$(H_+ \phi)_i := -\phi_{i+1} + 2\phi_i - \phi_{i-1} + \lambda \phi_i - (\sigma+1)|G_i|^{2\sigma} \phi_i. \quad (24)$$

Note that the Lagrangian multiplier has been scaled out, and solutions exist for continuous values of $\lambda = \eta^2$. Furthermore, for a finite chain the existence of the minimum follows from the fact that W is bounded from below for fixed I . For completeness and later use we also present the second variation. Using the abbreviation $\delta \psi_n = a_n + i b_n$, a short calculation leads to

$$\delta^2 W = \sum_{i=-N}^N a_i (H_- a)_i + \sum_{i=-N}^N b_i (H_+ b)_i \geq 0, \quad (25)$$

where

$$\begin{aligned} (H_- \phi)_i &:= -\phi_{i+1} + 2\phi_i - \phi_{i-1} + \lambda \phi_i \\ &\quad - (2\sigma+1)(\sigma+1)|G_i|^{2\sigma} \phi_i \\ &= (H_+ \phi)_i - 2\sigma(\sigma+1)|G_i|^{2\sigma} \phi_i. \end{aligned} \quad (26)$$

For a finite system, the fact that the minimum of W (under the constraint $I = \text{const}$) is attained for some $G \equiv \{G_i\}$ is obvious. The situation is completely different for an infinite system. Then we need a compactness lemma which ensures the survival of the constraint $I = \text{const}$ for the minimizing sequence. Since this is an interesting point with important physical implications, we present in the following those steps which show which solitons are selected in an infinite chain by this minimization procedure. In Fig. 1 we have characterized the typical modes we have in mind: they may have even or odd parities, and their centers may be on-site or intersite, respectively. Note also that only those with a low number of nodes (0 and 1) are shown.

A. Even parity ground state solutions

First we should note that W is bounded from below, $W \geq 0$. Then, a minimizing sequence $\psi^{(n)}$, $n=0,1,2,\dots$ exists. We use the notation $\psi^{(n)} \equiv \{\psi_i^{(n)}, i=0,\pm 1,\pm 2,\dots\}$ for each n , and we can choose a weakly convergent subsequence

$$\psi^{(n)} \rightharpoonup \psi \quad \text{and} \quad W^{(n)} \equiv W(\psi^{(n)}) \rightarrow \inf_{\varphi} W(\varphi) \quad \text{for } n \rightarrow \infty. \quad (27)$$

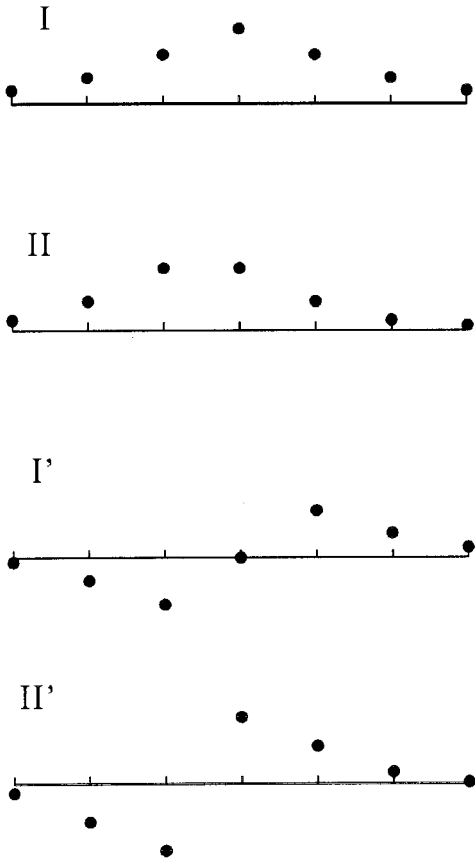


FIG. 1. Sketches of even parity (I, maximum on-site; II, maximum intersite) and odd parity (I', zero on-site; II', zero intersite) solutions.

Note that we have not yet proven $W(\psi) = \inf W$, i.e., that the minimum of W will be attained by ψ . The purpose of the next steps is to show under which conditions the infimum will be attained.

We can assume that the weakly convergent subsequence consists of non-negative elements $\psi_i^{(n)} \geq 0$, $i=0, \pm 1, \pm 2, \dots$ for $n=0, 1, 2, \dots$. The reason is

$$W(|\phi|) \leq W(\phi). \quad (28)$$

Moreover, we can even work with only positive elements $\psi_i^{(n)} > 0$ since it is straightforward to show that to each $\psi^{(n)}$ with zero element(s) a corresponding one with only positive elements and a lower value $W(\psi^{(n)})$ can be constructed. The idea is the following: Let us assume $\psi_{i-1}^{(n)} > 0$, $\psi_i^{(n)} = 0$, and $\psi_{i+1}^{(n)} \geq 0$ for some index i and fixed n . Then define

$$\tilde{\psi}_\mu^{(n)} := \psi_\mu^{(n)} / (1 + \epsilon^{2\sigma+2})^{1/2\sigma+2} \quad \text{for } \mu \neq i, \quad (29)$$

$$\tilde{\psi}_i^{(n)} = \epsilon / (1 + \epsilon^{2\sigma+2})^{1/2\sigma+2} > 0. \quad (30)$$

Obviously, $\tilde{I}^{(n)} = I^{(n)}$, where the superscript indicates that we evaluate Eq. (20) for $\tilde{\psi}^{(n)}$ (and $\tilde{\psi}^{(n)}$, respectively), and

$$\tilde{W}^{(n)} < W^{(n)} \quad \text{for } \epsilon > 0 \quad \text{and } \epsilon \rightarrow +0. \quad (31)$$

We have thus proven that a minimizing sequence with strictly positive elements $\psi_i^{(n)} \rightarrow \psi_i$ exists. Now let us have a look at the constraint $I = \text{const}$. The latter is an absolute convergent series for each element $\psi^{(n)}$. Thus we can rearrange the summations in Eq. (20) without changing the value of I . Let us do this such that

$$\psi_j^{(n)} \leq \psi_i^{(n)} \quad \text{for } |j| \geq i. \quad (32)$$

From here it will follow $\psi_j \leq \psi_i$ for $|j| \geq i$. In other words, we consider distributions with a single maximum. The latter can appear either for $i=0$, when the symmetric solutions are centered on-site, or at $i=0$ and $i=1$, for intersite centered solutions. The question is what happens to the value of W during such a rearrangement of the elements $\psi_j^{(n)}$ of $\psi^{(n)}$. One can prove that W attains a lower value after rearrangement. In other words, single maximum solutions correspond to the minimal value of W .

Having in mind this property of the minimizing sequence we can show the survival of the constraint I in the limiting process $\psi^{(n)} \rightarrow \psi$. Normalization

$$N_0^2 = \sum_{j=-\infty}^{\infty} |\psi_j^{(n)}|^2 \geq \sum_{j=1}^m |\psi_j^{(n)}|^2 \geq m(\psi_m^{(n)})^2 \quad (33)$$

leads to the estimate

$$(\psi_m^{(n)})^2 \leq \frac{N_0^2}{|m|} \quad \text{for } |m| \geq 1. \quad (34)$$

Thus we find for the ‘‘rest’’ defined by

$$I^{(n)} = \sum_{i=-m}^m |\psi_i^{(n)}|^{2\sigma+2} + R^{(n)}(m) \quad (35)$$

the estimate

$$R^{(n)}(m) \leq 2N_0^{2\sigma+2} \sum_{|k| > |m|} \frac{1}{|k|^{2\sigma+2}} \equiv f(m), \quad (36)$$

i.e., an upper bound independent on n . In addition, the upper bound tends to zero for large m ,

$$f(m) \rightarrow 0 \quad \text{for } m \rightarrow \infty. \quad (37)$$

Therefore,

$$\sum_{i=-m}^m |\psi_i^{(n)}|^{2\sigma+2} \rightarrow \sum_{i=-m}^m |\psi_i|^{2\sigma+2} \quad \text{for } n \rightarrow \infty \quad (38)$$

and any fixed m . In conclusion, the constraint survives (being equivalent to the existence of a compactness lemma) and the minimum of the variational principle will be attained by some distribution $\psi \equiv G$. Thus, we can find the even parity ground states by the variational principle which has been formulated above.

B. Odd parity solutions

One might be tempted to proceed for odd parity ground states (with only one zero either on-site or intersite) by using the same variational principle in the subspace of odd func-

tions (applying an additional boundary condition, e.g., $G_0 \equiv \psi_0 = 0$). Odd parity means for on-site centered solutions (which are considered in the following)

$$G_i = -G_{-i} \text{ for } i \geq 0, \quad (39)$$

when $G_0 = 0$; the condition can be easily modified for an intersite node with $G_0 = -G_1$. In the following we show that the minimum of W , with the constraint $I = \text{const}$, will not be attained by some function φ , i.e., in the notation of Sec. II A no function φ exists such that $W(\varphi) = \inf W$ for odd parity solutions (39).

The proof is indirect (by *conductio ad absurdum*). Let us assume that for $\psi^{(n)} \rightarrow \psi$

$$W(\psi^{(n)}) \rightarrow \inf_{\varphi} W(\varphi) = W(\psi) \quad (40)$$

is true. Without loss of generality we can assume $\psi_1 \equiv G_1 > 0$ (and $\psi_0 = 0$ for an on-site node). Now compare with the value \tilde{W} which is obtained by using instead of ψ the elements

$$\tilde{\psi}_0 = \psi_0, \quad (41)$$

$$\tilde{\psi}_1 = -\tilde{\psi}_{-1} \equiv f\epsilon, \quad (42)$$

$$\tilde{\psi}_i = f\psi_{i-1} \text{ for } i > 1, \quad (43)$$

$$\tilde{\psi}_i = f\psi_{i-1} \text{ for } i < -1. \quad (44)$$

They yield $\tilde{I} = I$ if

$$f^{2\sigma+2} [2\epsilon^{2\sigma+2} + I] = I, \quad (45)$$

i.e., for $\epsilon > 0$ we have to choose $f < 1$ accordingly. Now it is straightforward to calculate

$$\tilde{W} < W \text{ for } \epsilon \ll 1. \quad (46)$$

It is clear that the procedure (41)–(44) leads to a lower value of W which contradicts our assumption (40). Thus, for odd parity modes the infimum of the variational principle cannot be attained by some distribution ψ . This implies that, if at all, the existence of the odd parity solutions has to be proven by some other means. In the next section we present a simple method to calculate stationary solutions of even or odd parity, also with various numbers of nodes.

III. GENERATING FUNCTIONS FOR FAMILIES OF STATIONARY SOLUTIONS

We now outline a general procedure to construct stationary solutions. Consider the difference equation

$$\begin{aligned} & -F(x+1) + 2F(x) - F(x-1) + \lambda F(x) \\ & = (\sigma+1)[F(x)]^{2\sigma+1}, \quad -\infty < x < +\infty, \end{aligned} \quad (47)$$

with the boundary condition

$$F(x) \rightarrow 0 \text{ for } x \rightarrow \infty, \quad (48)$$

where x is a continuous variable. If this difference equation has a solution $F(x)$ for all x , then

$$G_i = F(\xi+i) \quad -\infty < i < \infty, \quad i \text{ integer}, \quad (49)$$

is obviously a solution of Eq. (13) for arbitrary real ξ . Note that even if $F(x)$ is not localized for $x \rightarrow -\infty$ one can construct G_i with $G_i \rightarrow 0$ for $i \rightarrow -\infty$ by using the symmetries of the discrete equation (13). This will be done choosing appropriate values for ξ .

A. Existence of solutions

First, the existence of solutions to Eq. (47) will be proven by making use of the formula

$$F(x) = e^{-\delta x} - \frac{\sigma+1}{\sinh(\delta)} \sum_{j=1}^{\infty} [F(x+j)]^{2\sigma+1} \sinh(\delta j), \quad (50)$$

where δ is determined via the ansatz $F(x) \sim e^{-\delta x}$ in the linear regime $x \rightarrow \infty$, i.e., with $\eta = \sqrt{\lambda}$:

$$\frac{\delta}{\sinh \frac{\delta}{2}} = \frac{\eta}{2}. \quad (51)$$

Two facts are important: (i) The solution of Eq. (50) obeys Eq. (47). (ii) It is sufficient to prove the existence of a solution to Eq. (50) for $[x_0, \infty)$, where x_0 is some large x -value. Then rewriting Eq. (47) as

$$F(x) = -F(x+2) + F(x+1) \{ \lambda + 2 - (\sigma+1)[F(x+1)]^{2\sigma} \}, \quad (52)$$

we can extend the existence region to any finite $x < x_0$, which will be needed for the construction of solutions to Eq. (13) by symmetry arguments in the following subsection.

We shall show now that the Volterra type equation (50) can be solved by iteration,

$$F_{n+1}(x) = e^{-\delta x} - \frac{\sigma+1}{\sinh(\delta)} \sum_{j=1}^{\infty} [F_n(x+j)]^{2\sigma+1} \sinh(\delta j), \quad (53)$$

with $F_0 \equiv e^{-\delta x}$.

It is straightforward to show that

$$F_1(x) > 0 \text{ for } x > x_0, \quad (54)$$

where x_0 is a (large) x -value to be determined appropriately. We have

$$F_1(x) = F_0(x) - \frac{(\sigma+1)e^{-(2\sigma+1)\delta x}}{\sinh(\sigma\delta)} \frac{1}{4\sinh[(\sigma+1)\delta]}. \quad (55)$$

From here also follows

$$F_1 < F_0. \quad (56)$$

For large $x > x_0$, we can write

$$|F_1(x) - F_0(x)| < \epsilon^1 F_0(x). \quad (57)$$

Let us consider (54), (56), and (57) as the first step within a proof by complete induction. It is straightforward to show that from

$$F_n > 0, \tag{58}$$

$$F_{n+1} \leq F_n, \tag{59}$$

and

$$|F_{n+1} - F_n| \leq \epsilon^{n+1} F_0 \leq \epsilon^{n+1} e^{-\delta x_0} \tag{60}$$

follows the next step

$$F_{n+1} > 0, \tag{61}$$

$$F_{n+2} \geq F_{n+1}, \tag{62}$$

$$|F_{n+2} - F_{n+1}| \leq \epsilon^{n+2} F_0 \leq \epsilon^{n+2} e^{-\delta x_0}, \tag{63}$$

provided x is large enough. Note that in (62) the inequality sign has reversed its direction. But this is exactly what we expected. For the general proof it does not cause any difficulties. We only have to make the distinction whether n is even or odd.

Having outlined the steps necessary to prove the alternating and converging behavior for large x , we can use Eq. (47) itself to uniquely find the values at lower x .

Now we briefly comment on the limiting function $F(x)$,

$$F_n(x) \rightarrow F(x) \text{ for } n \rightarrow \infty, \tag{64}$$

which should satisfy Eq. (50). It is quite straightforward to show that $F_n(x) = F(x) + \varphi_n(x)$ leads via (53) to Eq. (50) where on the right-hand side appears an additional ‘‘rest’’ R_n . However, the latter will vanish in the limit $n \rightarrow \infty$ by the estimates presented above. Due to (60) and (63) the convergence of F_n is uniform in $[x_0, \infty)$, and thus in Eq. (53) the summation commutes with the limit $n \rightarrow \infty$ for $x \geq x_0$.

Moreover, it is quite trivial to show that (50) satisfies (47). For the demonstration we only have to insert (50) into (47).

B. Construction of families of symmetric solutions

We have solved Eq. (47) with vanishing boundary conditions for $x \rightarrow +\infty$. Typical results are shown in Fig. 2. Starting from the asymptotic solution (in the linear regime) the numerical evaluation is quite simple, and one is not faced with any numerical problems. Of course, the numerics will fail for $x \rightarrow -\infty$, but, as we shall show below, that behavior is not needed for the determination of most members of the families of solutions.

The general form of the generating function is quite surprising at first glance. It has an oscillatory behavior, which allows us to construct several types of solutions to Eq. (13) in the form $G_j = F(j + \xi)$ [see (49)], with properly chosen ξ values. The oscillatory behavior, which is essential for the following conclusions, has its origin in the nonintegrability of Eq. (4). As has been mentioned already, the stationary solutions of Eq. (4) [see Eq. (13)] are related to the generalized standard mapping (14), (15), and Eq. (47) is the continuous analog of Eq. (13). The hyperbolic fixed point (0,0) of the mapping (14),(15) has a stable (W_s) and an unstable

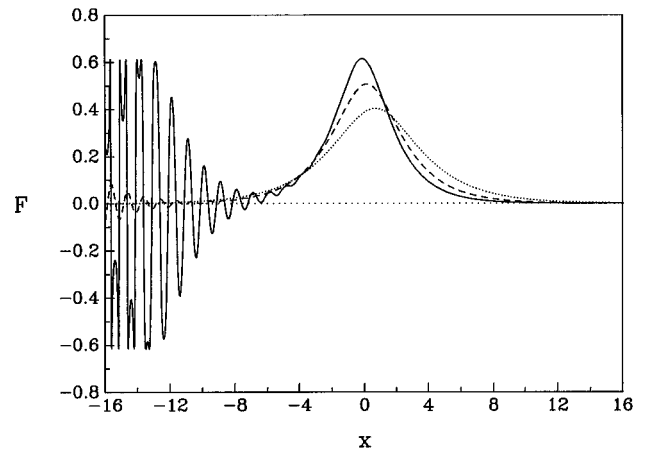


FIG. 2. Generating functions (DNS equation) for $\sigma=1$, η equal to 0.4 (dotted line), 0.5 (broken line), and 0.6 (solid line), respectively.

(W_u) manifold. Homoclinic points are the intersections of W_u and W_s , and it is known that in general the curves W_u and W_s form an extremely complex network. The generating function, being nonoscillatory and well-behaved on one side (e.g., for $x \rightarrow +\infty$ in Fig. 2) reveals this behavior. We have tested this interpretation by comparing with the integrable Ablowitz-Ladik equation, and, indeed, in that integrable case the generating function is nonoscillatory in the whole area. More on this interesting aspect will be published elsewhere.

By construction, G_i defined by Eq. (49) is a solution of Eq. (13) for any ξ . Since $G(x)$ is not vanishing for $x \rightarrow -\infty$, G_i will not fulfill the boundary conditions for arbitrary ξ . The way we suggest to construct localized solutions for $i \rightarrow -\infty$ is to use the following symmetry properties of the basic Eq. (13):

$$G_{-1} = G_1 \rightarrow G_{-i} = G_i \text{ for all } i, \tag{65}$$

$$G_{-1} = G_0 \rightarrow G_{-i} = G_{i-1} \text{ for all } i, \tag{66}$$

$$G_{-1} = -G_1 \rightarrow G_{-i} = -G_i \text{ for all } i, \tag{67}$$

$$G_{-1} = -G_0 \rightarrow G_{-i} = -G_{i-1} \text{ for all } i, \text{ respectively.} \tag{68}$$

First let us look for symmetric solutions being centered on-site, as depicted schematically on top of Fig. 1. We define the auxiliary function

$$F_{so}(x) := F(x+1) - F(x-1). \tag{69}$$

This function is plotted in Fig. 3, and its zero points ξ_i^{so} are easy to determine,

$$F_{so}(\xi_k^{so}) = 0. \tag{70}$$

Specifying the index k (out of the family of zeros for $k=0,1,2,\dots$) we define

$$G_j^{(k)} = F(\xi_k^{so} + j) \text{ for } j \geq 0, \tag{71}$$

$$G_j^{(k)} = G_{-j}^{(k)} \text{ for } j \leq 0. \tag{72}$$

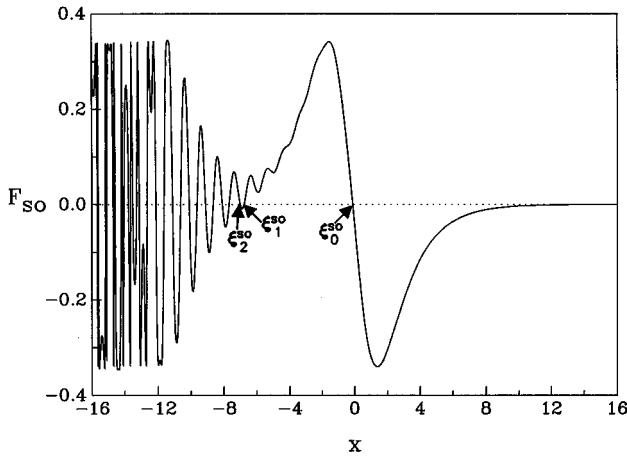


FIG. 3. Auxiliary function F_{so} (DNS equation for symmetric solutions centered on-site) for $\sigma=1$, $\eta=\sqrt{\lambda}$ equal to 0.6. The first three zeros of F_{so} are marked.

$G_j^{(k)}$ defined by Eq. (71) is a solution of Eq. (13) since $F(x)$ fulfills Eq. (47). Due to (70) one has $G_1^{(k)}=G_{-1}^{(k)}$, and therefore Eq. (72) follows by using Eq. (65).

Now it is clear that due to the existence of a whole set of zeros ξ_k^{so} of F_{so} , a whole family of on-site symmetric discrete localized solutions exists. Typical examples are shown in Fig. 4.

Next, symmetric solutions with intersite centers are calculated. We define

$$F_{si}(x) := F(x) - F(x-1) \tag{73}$$

and solve for

$$F_{si}(\xi_k^{si}) = 0, \text{ for } k=0,1,2, \dots \tag{74}$$

The solutions G_j are obtained from

$$G_j^{(k)} = F(\xi_k^{si} + j) \text{ for } j \geq 0, \tag{75}$$

$$G_j^{(k)} = G_{-j-1}^{(k)} \text{ for } j \leq -1. \tag{76}$$

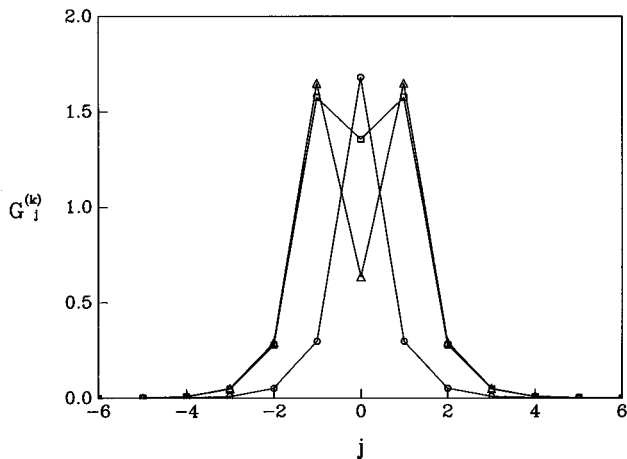


FIG. 4. Symmetric on-site centered DNS solutions for $\sigma=1$, $\eta=2$, and k equal to 0(\circ), 1(\diamond), and 2(\triangleleft), respectively.

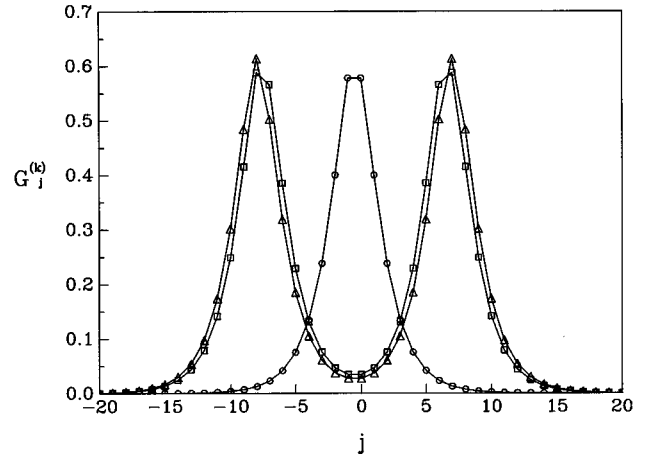


FIG. 5. Symmetric intersite centered DNS solutions for $\sigma=1$, $\eta=0.6$, and k equal to 0(\circ), 1(\square), and 2(\triangle), respectively.

Typical examples are shown in Fig. 5.

The third type of solutions, being antisymmetric and centered on-site, follows by

$$F_{ao}(x) := F(x), \tag{77}$$

$$F_{ao}(\xi_k^{ao}) = 0, \text{ } k=0,1,2, \dots, \tag{78}$$

$$G_j^{(k)} = F(\xi_k^{ao} + j) \text{ for } j \geq 0, \tag{79}$$

$$G_j^{(k)} = -G_{-j}^{(k)} \text{ for } j \leq 0. \tag{80}$$

These solutions are shown in Fig. 6. Finally, we determine the family of antisymmetric and intersite centered solutions. They follow from

$$F_{ai}(x) := F(x) + F(x-1), \tag{81}$$

$$F_{ai}(\xi_k^{ai}) = 0, \text{ } k=0,1,2, \dots \tag{82}$$

It is straightforward to construct

$$G_j^{(k)} = F(\xi_k^{ai} + j) \text{ for } j \geq 0, \tag{83}$$

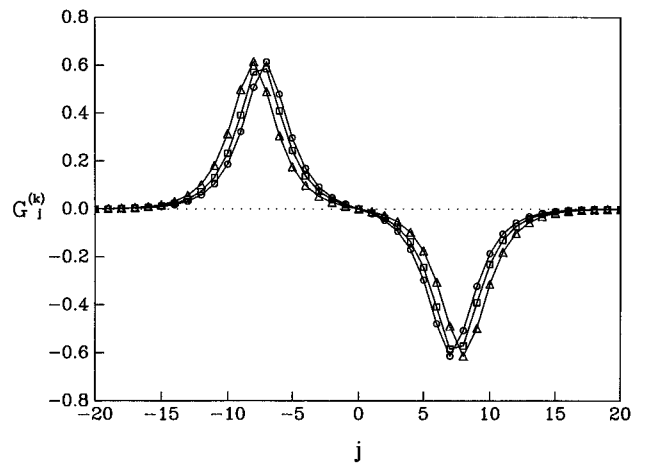


FIG. 6. Antisymmetric on-site centered DNS solutions for $\sigma=1$, $\eta=0.6$, and k equal to 0(\circ), 1(\square), and 2(\triangle), respectively.

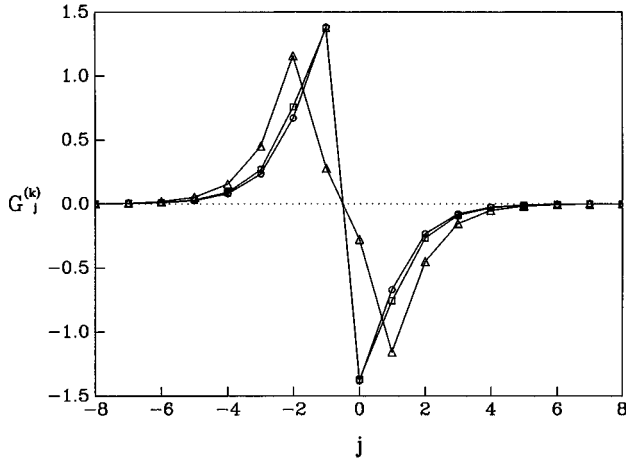


FIG. 7. Antisymmetric intersite centered DNS solutions for $\sigma=1$, $\eta=1.145$, and k equal to 0(\circ), 1(\square), and 2(\triangle), respectively.

$$G_j^{(k)} = -G_{-j-1}^{(k)} \text{ for } j \leq 0. \quad (84)$$

Typical members of the family of solutions are depicted in Fig. 7.

This completes the discussion on stationary localized solutions of the discrete nonlinear Schrödinger equation. The stability of these solutions is considered next.

IV. STABILITY CONSIDERATIONS

We now go back to the time-dependent Eq. (4) in order to discuss the dynamical behavior of the just found stationary solutions in the presence of perturbations. Introducing

$$\psi_j = (G_j + a_j + ib_j)e^{i\lambda t}, \quad (85)$$

and using the operators H_+ and H_- defined in Eqs. (24) and (26), respectively, we find in the linear limit

$$\partial_t^2 a_j = -(H_+ H_- a)_j. \quad (86)$$

A. Definiteness properties of the operators

In Sec. II A we have shown that *symmetric* ground states realize the minimum of W under the constraint $I = \text{const}$. A similar calculation as that leading to Eq. (25) (for the finite-dimensional case) gives in the infinite-dimensional case $\delta^2 W \geq 0$, i.e.,

$$\sum_j s_j (H_- s)_j \geq 0 \quad (87)$$

for

$$\sum_j s_j G_j^{2\sigma+1} = 0. \quad (88)$$

It is important to note that these relations are only true provided the disturbances have the same symmetry property as the *even* ground state (centered either on-site or intersite).

For odd disturbances (87) was not proved in Sec. II A. Note also that from the definitions of the operators H_+ and H_- we have

$$\sum_j s_j (H_- s)_j \leq \sum_j s_j (H_+ s)_j. \quad (89)$$

From here it follows that H_+ is positive semidefinite for the symmetric ground state ($k=0$) solutions (being either centered on-site or intersite). The argument is the following. Assume that H_+ has a negative eigenvalue. If the corresponding eigensolution e_j is orthogonal to $G_j^{2\sigma+1}$ the contradiction to

$$\delta^2 W = \sum_j a_j (H_- a)_j + \sum_j b_j (H_+ b)_j \geq 0 \quad (90)$$

is obvious [let $a_j = b_j = e_j$ in Eq. (90) and make use of inequality (89)]. If the eigensolution e_j is not orthogonal to $G_j^{2\sigma+1}$ we construct

$$f_j := G_j - \frac{\sum_i G_i^{2\sigma+2}}{\sum_i e_i G_i^{2\sigma+1}} e_i, \quad (91)$$

which is orthogonal to $G_j^{2\sigma+1}$. Since $(H_+ G)_j = 0$, we can use similar arguments as above to find a contradiction.

Now let us discuss the spectral properties of H_- . H_- has at least one negative eigenvalue since

$$\sum_j G_j (H_- G)_j < 0 \quad (92)$$

holds. For (on-site as well as intersite centered) symmetric ground states, however, H_- has only one negative eigenvalue. Let us assume that two negative eigenvalues μ_1 and μ_2 exist; we denote the corresponding (orthogonal) eigensolutions by e_j and f_j , respectively, and define

$$r_j := \delta_1 e_j + \delta_2 f_j. \quad (93)$$

The coefficients $\delta_1 \neq 0$ and $\delta_2 \neq 0$ are determined by the condition

$$\sum_j r_j G_j^{2\sigma+1} = 0. \quad (94)$$

This is possible since $\sum_j e_j G_j^{2\sigma+1} \neq 0$ and $\sum_j f_j G_j^{2\sigma+1} \neq 0$ can be assumed; otherwise Eqs. (87) and (88) lead to an immediate contradiction. But now also

$$\sum_j r_j (H_- r)_j < 0 \quad (95)$$

will follow which, on the other hand, is forbidden via Eq. (94).

B. Stability criterion

Coming back to the dynamical equation, we know that for symmetric ground state solutions G_j of types I or II (see Fig.

1), (i) H_+ is positive semidefinite with $(H_+G)_j=0$; (ii) H_- has only one negative eigenvalue, and $\sum_j G_j(H_-G)_j < 0$.

Under these conditions it is well-known that instability occurs provided

$$\Gamma^2 := \sup_{C(\varphi)} \frac{-\sum_j \varphi_j (H_- \varphi)_j}{\sum_j \varphi_j (H_+^{-1} \varphi)_j} > 0, \quad (96)$$

where the supremum is determined for all possible φ_j under the condition

$$C(\varphi): \sum_j \varphi_j G_j = 0. \quad (97)$$

Of course, the occurrence of instability depends on the further properties of H_- . If, and only if, under the condition (97) the expression $\sum_j \varphi_j (H_- \varphi)_j$ can become negative, instability will occur. Easier to calculate for the latter behavior is the condition

$$\sum_j G_j (H_-^{-1} G)_j > 0. \quad (98)$$

The existence of $H_-^{-1} G$ will become obvious later. We shall comment on that as well as on the evaluation of the criterion in Sec. IV C. Before doing so let us complete the general stability criterion (96) by a complementary one which can be derived in the case when H_- has only one negative eigenvalue. It reads

$$\gamma^2 := \inf_{\varphi} \frac{\sum_j \varphi_j (H_- H_+ H_- \varphi)_j}{\sum_j \varphi_j (H_- \varphi)_j} > 0 \quad (99)$$

for instability.

C. The N -theorem

The variational principles (96) and (99) can be evaluated numerically by adopting a Galerkin approximation and determining the expansion coefficients by an appropriate minimization scheme. More basic evaluations go back to Eq. (86) and determine the spectral properties of H_+ and H_- numerically. But a criterion like (98) is much simpler since it allows us to determine the stability properties by a straightforward summation. So let us prove (98) for instability first. We have

$$(H_- e)_j = -|\mu| e_j, \quad (100)$$

when e_j is the eigensolution corresponding to the (only) one negative eigenvalue μ of H_- , and $\sum_j G_j (H_- G)_j < 0$. Next we construct

$$\varphi_j := \frac{-\sum_i G_i (H_-^{-1} G)_i}{\sum_i e_i G_i} e_j + (H_-^{-1} G)_j. \quad (101)$$

Since G and e are ground states of the Schrödinger operators H_+ and H_- , respectively, the signs of G_i and e_i are independent of i . Thus the denominator in (101) cannot vanish.

Under the assumption (98) it is straightforward to prove that

$$\sum_j \varphi_j (H_- \varphi)_j < 0 \quad (102)$$

and

$$\sum_j \varphi_j G_j = 0, \quad (103)$$

i.e., $\Gamma^2 > 0$ according to the criterion (96).

On the contrary, if

$$\sum_j G_j (H_-^{-1} G)_j < 0 \quad (104)$$

no test distribution φ_j exists which makes $\Gamma^2 > 0$ (i.e., we have a stable situation). Let us prove this. We define

$$F_j := (H_-^{-1} G)_j \quad (105)$$

and split any test distribution in a part with index (\parallel) being parallel to e_j and a part with index (\perp) being perpendicular to e_j . Then we have

$$\sum_j \varphi_j (H_- \varphi)_j = -|\mu| \left[\sum_j \varphi_{\parallel j} \varphi_{\parallel j} + \sum_j \varphi_{\perp j} (H_- \varphi_{\perp})_j \right]. \quad (106)$$

In addition, from condition (97) we obtain

$$|\mu| \sum_j \varphi_{\parallel j} F_{\parallel j} = \sum_j \varphi_{\perp j} (H_- F_{\perp})_j, \quad (107)$$

whereas condition (104) implies

$$\sum_j F_{\perp j} (H_- F_{\perp})_j < |\mu| \sum_j F_{\parallel j} F_{\parallel j}. \quad (108)$$

Finally we use the Schwarz inequality

$$\left[\sum_j \varphi_{\perp j} (H_- \varphi_{\perp})_j \right] \left[\sum_j F_{\perp j} (H_- F_{\perp})_j \right] \geq \left[\sum_j \varphi_{\perp j} (H_- F_{\perp})_j \right]^2. \quad (109)$$

With these ingredients we can estimate (from below) the second term on the right-hand side of Eq. (106). The results can be easily combined with the first term on the right-hand side of Eq. (106) when

$$\left[\sum_j \varphi_{\parallel j} F_{\parallel j} \right]^2 = \left[\sum_j \varphi_{\parallel j} \varphi_{\parallel j} \right] \left[\sum_j F_{\parallel j} F_{\parallel j} \right] \quad (110)$$

is used. Then finally we arrive at

$$\sum_j \varphi_j (H_- \varphi)_j \geq 0. \quad (111)$$

Thus, for (104) we have no instability. It should be noted that under condition (104)

$$L = W - (\sigma + 1)I - W_s + (\sigma + 1)I_s, \quad (112)$$

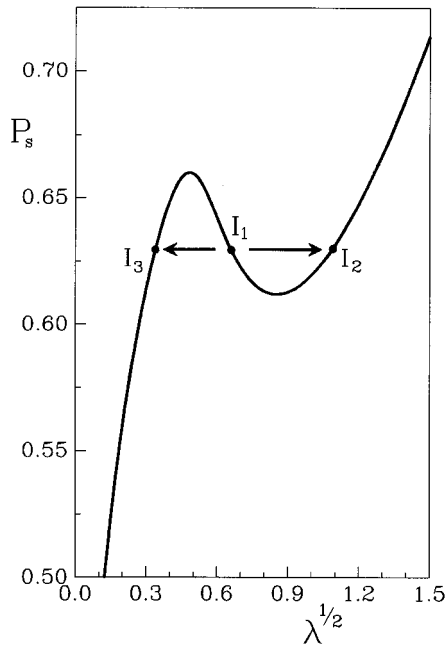


FIG. 8. Excitation density P_s vs square root of frequency shift λ of stationary solutions of type I for $\sigma=1.6$. The monotonically growing parts of the curve belong to stable states.

where the subscript s denotes values being calculated for the stationary solutions, can be used as a Liapunov functional for stability. The main steps of that proof are those presented above.

Our final point is to rewrite (98) so that it can easily be evaluated.

Since

$$\left(H_- \frac{\partial}{\partial \lambda} G \right)_j = -G_j \quad (113)$$

we can reformulate (98) as

$$\frac{\partial}{\partial \lambda} \sum_j G_j^2 < 0 \Rightarrow \text{instability for even perturbations.} \quad (114)$$

Let us comment once more on an additional restriction. The definiteness properties being used here assume symmetric (even parity) ground states with centers either on-site or intersite. Thus the criterion (114) gives an answer to the question of the (initial time) dynamics of an even ground state of type I or II (see Fig. 1) with respect to even perturbations, i.e., perturbations of the same parity.

Now we briefly present the results of the evaluation of (114). Let us denote the excitation density in the chain by

$$P_s = \sum_j G_j^2. \quad (115)$$

As long as P_s is increasing with λ , the ground state is stable with respect to even perturbations. A typical example for the evaluation of the criterion is shown in Fig. 8. This graph is for a fixed σ -value ($\sigma=1.6$ in Fig. 8) and for type-I solutions. The monotonically growing parts of the curve belong

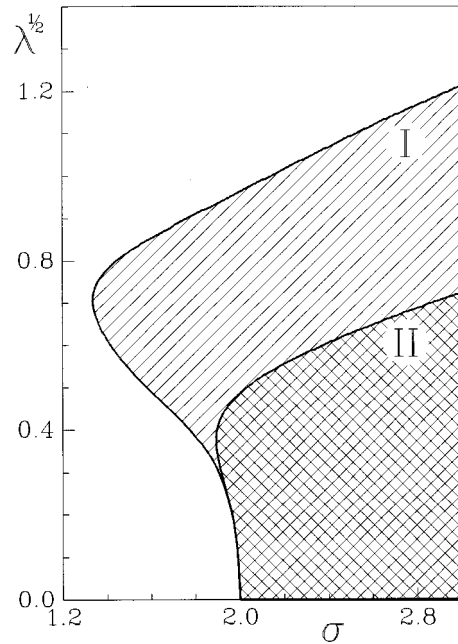


FIG. 9. Stability diagram of solutions of types I and II with respect to parity-conserving (even) perturbations. The solitary waves are unstable in the hatched regions to the right of the curves labeled I and II, respectively.

to stable states. Repeating the calculations for other σ -values and also for type-II solutions, we get the information about the stability behavior in the (σ, λ) -plane. The results are depicted in Fig. 9. We have stable and unstable regimes which are separated in Fig. 9 by the border lines named I (for type-I solutions) and II (for type-II solutions), respectively. The localized ground states of types I or II are unstable in the right neighborhoods of the curves marked I or II, respectively, i.e., in the hatched areas. One can see that the discreteness changes the critical value (σ_{cr}) of σ that separates stable and unstable solitons. In the continuum limit $\sigma_{cr}=2$. Here we find $\sigma_{cr} \approx 1.4$. Perturbations can have other symmetry properties, i.e., the stationary solutions can be even more unstable, and then we need additional information which usually is only available through numerical calculations. To close this last gap is the purpose of the next subsection.

D. Arbitrary perturbations

In the case of ground states of types I or II the stability investigations with respect to arbitrary perturbations can be based on a discussion of the spectral properties of H_- . Note that in analogy to the continuum case, also for the discrete case theorems are known which relate the forms of the eigen-solutions to the hierarchy of eigenvalues. But for the more general cases, i.e., all the solutions constructed by the generating functions, we have to rely on (simple) numerical procedures [30] to determine the spectral behaviors of H_+ and H_- . We do not discuss more special cases separately but summarize the results.

For ground states of type I (symmetric even parity, no nodes, centered on-site) no additional negative eigenvalue of H_- enters the stability considerations, compared to the situ-

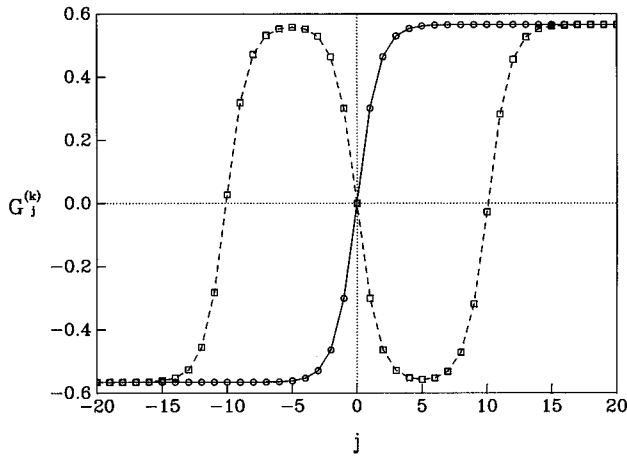


FIG. 10. Antisymmetric on-site centered solutions of the DNKG equation for $\sigma=1$, $\eta=0.8$, and k equal to 0(\circ) and 1(\square), respectively.

ation discussed in Sec. IV C. Thus, curve I of Fig. 9 is the exact (and completely general) stability boundary.

The situation is different for ground states of type II (symmetric with even parity, no nodes, centered intersite). These solutions are always unstable with respect to odd perturbations.

Other members of the families starting from types I or II, respectively (i.e., those being constructed from F_{so} and F_{si} , respectively) are in general not stable, although for some of the solutions with even parity the possible upper limits for the growth rates are so small that physically those solutions can be considered as quasistable. To be more concrete, in Fig. 4, the ground state solution (\circ) is stable whereas all the other even symmetric solutions, centered on-site (marked by \square and \triangle in Fig. 4), are unstable. On the contrary, all the even symmetric solutions, centered intersite, and shown in Fig. 5 ($\circ, \square, \triangle$) are unstable. Note again that some of the so-called unstable solutions have extremely small growth rates so that from the application point of view they may be called quasistable.

Next we turn to the odd symmetric solutions of the DNS, shown in Fig. 6 (centered on-site) and Fig. 7 (centered intersite). Our analysis has shown that all these solutions are unstable. The calculated growth rates are significant so that there are no quasistable solutions.

V. KLEIN-GORDON CHAINS

In the preceding sections we have outlined the general methods for proving the existence and stability of discrete solitary solutions in nonlinear chains. Specific results have been presented for the DNS equation (4). Now we demonstrate the power of the proposed procedure by applying it to the discrete nonlinear Klein-Gordon (DNKG) equation

$$\partial_t^2 U_j - (U_{j+1} - 2U_j + U_{j-1}) \pm \eta^2 U_j \mp (\sigma + 1) U_j^{\sigma+1} = 0, \quad (116)$$

where in the following we shall discuss, in close similarity to the previous considerations, only the lower sign. Stationary solutions $U_j = G_j$ obey the equation

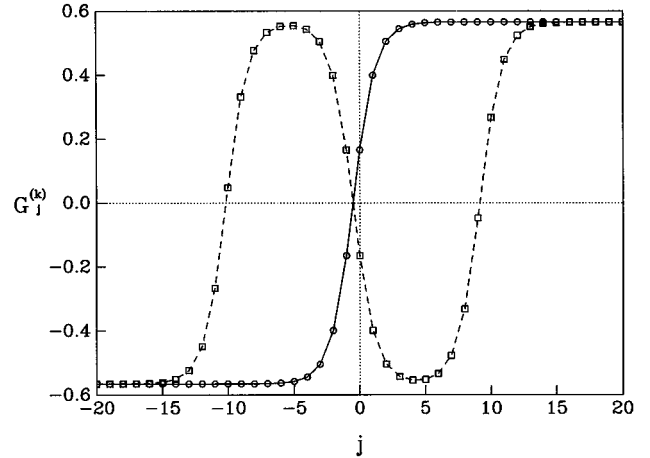


FIG. 11. Antisymmetric intersite centered solutions of the DNKG equation for $\sigma=1$, $\eta=0.8$, and k equal to 0(\circ) and 1(\square), respectively.

$$(H_+ G)_j = 0 \quad (117)$$

in strict analogy to Eq. (24). In contrast to the previous Schrödinger case, we apply the boundary condition

$$\lim_{j \rightarrow -\infty} G_j = -\frac{\eta}{\sqrt{2}}. \quad (118)$$

With slight but obvious modifications we can prove the existence of a generating function [see Eq. (47)] and determine stationary solutions of Eq. (116). Typical examples are shown in Figs. 10–13. Let us start with odd symmetry solutions being centered on-site. These belong to well-known kink-type distributions. Intersite centered kink-type solutions are shown in Fig. 11. Figures 12 and 13 belong to even symmetric solutions being either centered on-site or intersite, respectively. Note that in each of the figures only the first two types (out of a whole family) of solutions are shown.

Now we present stability results for discrete solitary waves of the DNKG equation. The ground state (\circ) solution shown in Fig. 10 (odd symmetry, centered on-site) is unstable. We can prove this by perturbing the stationary solution G_j in the form

$$U_j = G_j + g_j. \quad (119)$$

After linearization we obtain for g_j

$$\partial_t^2 g_j = -(H_- g)_j, \quad (120)$$

where H_- is defined in Eq. (26) (in the following we consider only $\sigma=1$). Note that Eq. (120) is much simpler than Eq. (86). We can easily determine the eigenvalues of H_- for each stationary solution. The results (instability for negative eigenvalues of H_-) are as follows.

As has been mentioned already, the ground state solution (\circ) shown in Fig. 10 (odd parity, centered on-site) is unstable. The same holds for the next member (\square) of the family. On the other hand, the ground state (\circ) shown in Fig. 11 (odd parity, centered intersite) is stable, whereas the next state (\square) is again unstable. It is also straightforward to de-

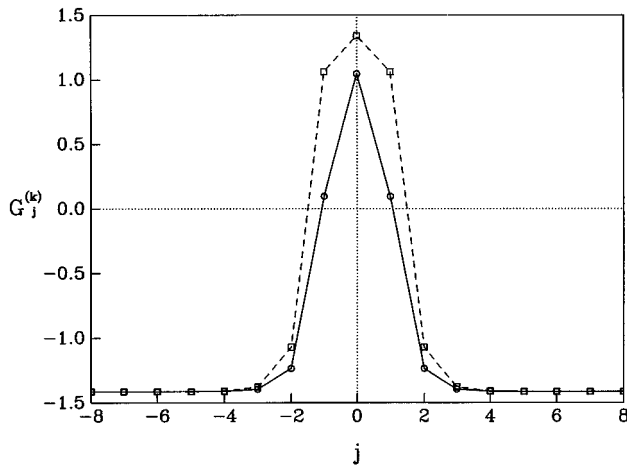


FIG. 12. Symmetric on-site centered solutions of the DNKG equation for $\sigma=1$, $\eta=2$, and k equal to 0(\circ) and 1(\square), respectively.

termine stationary even parity solutions of Eq. (116). Typical examples are shown in Fig. 12 (centered on-site) and Fig. 13 (centered intersite). In Fig. 12 the ground state (\circ) of the even symmetric on-site centered solitary distribution is unstable, whereas the next (\square) state is stable. On the other hand, the ground state (\circ) of the intersite centered solutions (see Fig. 13) is unstable whereas the next state (\square) is stable. We remind the reader that the solutions are “numbered” with respect to the zeros of the corresponding generating function; a “ground state” belongs to the first zero.

The analysis of the DNKG equation thus detects stable localized modes which might be useful in nonlinear transport mechanisms.

VI. SUMMARY AND OUTLOOK

In this paper we have discussed various possibilities to determine solitary solutions in discrete systems. The method, making use of generating functions, turns out to be powerful and constructive. We have applied it to two examples: the discrete nonlinear Schrödinger (DNS) equation and the discrete nonlinear Klein-Gordon (DNKG) equation. Further-

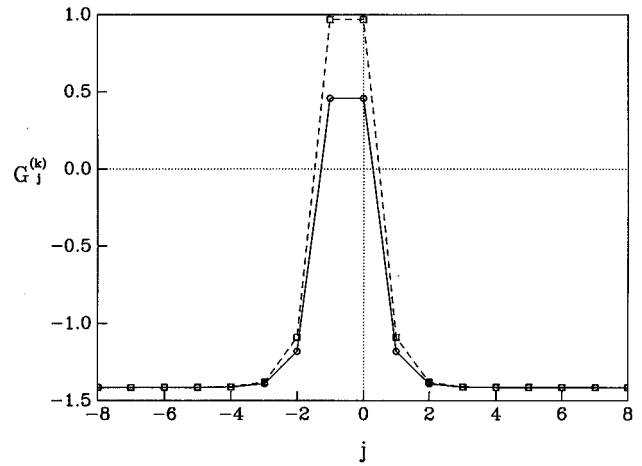


FIG. 13. Symmetric intersite centered solutions of the DNKG equation for $\sigma=1$, $\eta=2$, and k equal to 0(\circ) and 1(\square), respectively.

more, we have worked out variational principles for determining the stability properties. Besides the development of noteworthy methods, two physical results are most important. (i) The discrete DNS has a stronger tendency to form very localized states than its continuum version (with collapse). The critical nonlinearity parameter is significantly reduced. (ii) Additional states have been found. Especially for the DNKG, there are numerous *stable* ones which are of physical relevance. It is quite obvious that the methods being developed here can also be applied to other discrete systems.

Finally it should be noted that fully time-dependent simulations of Eqs. (4) and (116) have confirmed all the findings presented in this paper. The simulations also allow us to determine the nonlinear developments of the instabilities; however, their presentation is beyond the scope of the present paper.

ACKNOWLEDGMENTS

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